Josephson Current in S-FIF-S Junctions: Nonmonotonic Dependence on Misorientation Angle

Yu. S. Barash[1], I. V. Bobkova[1] and T. Kopp[2]
[1] *Lebedev Physical Institute, Leninsky Prospect 53, Moscow 119991, Russia*
[2] *Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany*

Spectra and spin structures of Andreev interface states in *S-FIF-S* junctions are investigated with emphasis on finite transparency and misorientation angle φ between in-plane magnetizations of ferromagnetic layers in a three-layer interface. It is demonstrated that the Josephson current in *S-FIF-S* quantum point contacts can exhibit a nonmonotonic dependence on the misorientation angle. The characteristic behavior takes place, if the π-state is the equilibrium state of the junction in the particular case of parallel magnetizations.

The dc Josephson effect in junctions with ferromagnetic interfaces exposes remarkable features which have been intensively studied in recent years theoretically [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17] and experimentally [18, 19]. Apart from interfaces with a fixed magnetization, considerable attention has been drawn also to more complicated cases, when the magnetization is spatially dependent inside the interface. An important particular model for this kind of interfaces is a three-layer *FIF*-interface, where two metallic ferromagnetic layers with in-plane magnetizations, making angle φ with each other, are separated by an insulating magnetically inactive interlayer [9, 10, 11, 14, 16]. In the present article we identify theoretically spectra and spin polarization of Andreev states bound to the three-layer *FIF*-constrictions with finite transmission, separating clean s-wave superconductors. Then we determine the Josephson current in the *S-FIF-S* quantum point contacts. This problem was not studied previously in the literature. In the dirty limit, considered in [9, 10, 16], Andreev bound states are fully destroyed. Considerations of Ref. 11 imply the absence of Andreev bound states in clean *S-FIF-S* junctions. This can be justified only for short superconductors, whose lengths are less than their coherence lengths. Spectra of Andreev states and the Josephson current in *S-FIF-S* junctions with $\varphi \neq 0$ have been found earlier only in the particular limit of fully transparent constriction which was characterized by the authors as a toy model [14].

The misorientation angle φ can be considered, in general, as a variable quantity. Let, for instance, the magnetization axis be pinned in one ferromagnetic layer, while in the other one there is an easy in-plane magnetization layer. Then one can vary the misorientation angle (keeping other parameters fixed) by applying an external weak magnetic field to the interface. We find that the Josephson current as a function of the misorientation angle φ manifests a characteristic nonmonotonic behavior, if, at $\varphi = 0$, the π-state is the equilibrium state of the junction.

For our analysis, we examine a smooth plane interface between two superconductors which consists of two layers of the same ferromagnetic metal separated by an insulating nonmagnetic barrier. Two identical ferromagnetic layers are characterized by their thickness l and internal exchange fields $|\boldsymbol{h}_{1,2}| = h$, which, being parallel to the layers, make an angle φ with each other.

The normal-state scattering $\mathcal{S}$ matrix is represented as $\mathcal{S} = S(1+\hat{\tau}_z)/2 + \widetilde{S}(1-\hat{\tau}_z)/2$, where the Pauli-matrices $\hat{\tau}_j$ are taken in particle-hole space and $\widetilde{S}(p_\parallel) = S^T(-p_\parallel)$. Each component $\hat{S}_{ij}$ in matrix $S = \|\hat{S}_{ij}\|$ $(i(j) = 1,2)$ is in its turn a matrix in spin space. Matrix $\hat{S}_{ii} = \begin{pmatrix} r_i^{\uparrow\uparrow} & r_i^{\uparrow\downarrow} \\ r_i^{\downarrow\uparrow} & r_i^{\downarrow\downarrow} \end{pmatrix}$ contains, in general, spin-dependent interface reflection amplitudes for normal-state quasiparticles in i-th half-space, while $\hat{S}_{ij} = \begin{pmatrix} d_{ij}^{\uparrow\uparrow} & d_{ij}^{\uparrow\downarrow} \\ d_{ij}^{\downarrow\uparrow} & d_{ij}^{\downarrow\downarrow} \end{pmatrix}$ with $i \neq j$ incorporates spin-dependent transmission amplitudes for normal-state quasiparticles from side j. For the interface potentials conserving particle current, the scattering matrix has to satisfy the unitarity condition: $\mathcal{S}\mathcal{S}^\dagger = 1$. If the interface Hamiltonian possesses time-reversal symmetry, one obtains an additional constraint on the scattering matrix: $S(\boldsymbol{p}_f, \boldsymbol{h}_{1,2}) = \hat{\sigma}_y S^T(-\underline{\boldsymbol{p}}_f, -\boldsymbol{h}_{1,2})\hat{\sigma}_y$ [3]. Assume, for simplicity, the exchange fields to be much smaller compared to the Fermi energies. For the diagonalization of the S_{11}-matrix we choose the z-axis along the magnetization in the first (left) ferromagnetic layer. Then the other S_{ij}-matrices are nondiagonal unless $\varphi = 0, \pi$:

$$\hat{S}_{21} = d \exp\left(\frac{i\Theta}{4}\left(\hat{\sigma}_y \sin\varphi + \hat{\sigma}_z \cos\varphi\right)\right) \exp\left(\frac{i\Theta}{4}\hat{\sigma}_z\right),$$

$$\hat{S}_{12} = d \exp\left(\frac{i\Theta}{4}\hat{\sigma}_z\right) \exp\left(\frac{i\Theta}{4}\left(\hat{\sigma}_y \sin\varphi + \hat{\sigma}_z \cos\varphi\right)\right),$$

$$\hat{S}_{11} = r \exp\left(i\frac{\Theta}{2}\hat{\sigma}_z\right),$$

$$\hat{S}_{22} = \tilde{r} \exp\left(i\frac{\Theta}{2} \left(\hat{\sigma}_y \sin\varphi + \hat{\sigma}_z \cos\varphi\right)\right) \ . \qquad (1)$$

Here $\Theta = \frac{4lh}{\hbar v_{f,x}}$. Quantities r, $\tilde{r}$ and d are the respective reflection and transmission amplitudes of the potential barrier V, satisfying the condition $rd^* = -d\tilde{r}^*$.

We carry out calculations within the quasiclassical theory of superconductivity, based on the equations for the so-called Riccati amplitudes or coherence functions [8, 20, 21]. Considering a quantum point contact with *FIF*-constriction, the order parameter is taken spatially constant. We include interface exchange fields in the quasiclassical boundary conditions. Since they imply, as usually, that all interface potentials are much larger than the superconducting order parameter [22], one should assume $|h_{1,2}| \gg \Delta$.

With the above normal-state $\mathcal{S}$ matrix we get *four branches of interface Andreev bound states*:

$$\varepsilon_{1,2} = |\Delta| \cos\frac{\Phi_{1,2}}{2} \ , \qquad \varepsilon_{3,4} = -|\Delta| \cos\frac{\Phi_{1,2}}{2} \ , \qquad (2)$$

where the quantities $\Phi_{1,2}(\chi, \Theta, \varphi)$ are defined as

$$\cos\Phi_{1,2}(\chi,\Theta,\varphi) = \cos\Theta - 2D\cos\Theta\sin^2\frac{\chi}{2} + \\ +2D\cos\chi\sin^2\frac{\Theta}{2}\sin^2\frac{\varphi}{2} \pm 2\sqrt{D}\sin\frac{\chi}{2}\sin\Theta\cos\frac{\varphi}{2}\times \\ \times\sqrt{1 - D\sin^2\frac{\chi}{2} + D\cos^2\frac{\chi}{2}\tan^2\frac{\Theta}{2}\sin^2\frac{\varphi}{2}} \ . \ (3)$$

Here, χ is the phase difference of the two superconductors. The energies ε_i $(i = 1, 2, 3, 4)$ implicitly depend on quasiparticle momentum directions via the parameter Θ and the transmission coefficient D.

For $\varphi = 0$ the spectra Eq. (3) reduce to those found in Ref. 12. In the particular case of antiparallel orientation of the left and the right magnetization $\varphi = \pi$, the spectra of Andreev interface states (2), (3) take the form

$$\varepsilon_1 = \varepsilon_2 = -\varepsilon_3 = -\varepsilon_4 = |\Delta|\sqrt{D\cos^2\frac{\chi}{2} + R\cos^2\frac{\Theta}{2}} \ . \qquad (4)$$

Being symmetric with respect to the transformation $\Theta \to -\Theta$, the spectrum (4) is doubly degenerated. In the limit of a nonmagnetic interface ($\Theta = 0$), our result, Eqs. (2) and (3), leads to a well known spectrum of spin-degenerate interface Andreev bound states [23, 24, 25, 26] $\varepsilon_B = \pm|\Delta|\sqrt{1 - D\sin^2(\chi/2)}$.

Quasiparticle spin is a qood quantum number in the BCS theory of superconductivity, if one can disregard spin-flip effects stimulated, for instance, by magnetic impurities, spin-orbit interactions or magnetically active interfaces. In the presence of a paramagnetic spin interaction with an externally applied magnetic field or an internal exchange field, spin degeneracy of quasiparticle states is lifted and only states with parallel or antiparallel spin-to-field orientations are still eigenstates of the problem. This can lead to effects having physics common with the Larkin-Ovchinnikov-Fulde-Ferrell state [27, 28] and, in particular, associated with opposite signs of the Zeeman terms for electrons forming a Cooper pair in singlet superconductors.

A Bogoliubov quasiparticle in the superconductor has well defined spin, although its electron and hole components are described with Zeeman terms of opposite signs. Also, an electron and its Andreev reflected partner (hole) at an interface, separating singlet superconductors and leading to no spin-flip processes, have identical spin orientations and opposite signs of Zeeman terms. With opposite velocity directions and electric charges, while in identical spin states, they carry jointly the electric supercurrent across the interface, but no equilibrium spin current. Hence, definite spin polarization of interface Andreev bound states is fully compatible with the fact that Cooper pairs in singlet supercoductors carry no spin current.

Andreev states bound to nonmagnetic interfaces are spin degenerated. For a ferromagnetic interface with uniformly oriented magnetization Andreev interface states are spin polarized, being parrallel or antiparallel to the magnetization. The ferromagnetic interface lifts spin degeneracy of the Andreev states, but still does not mix the spin-polarized channels, carrying the Josephson current [15]. This is not the case, however, if various orientations of magnetization are present in the interface, as this takes place in the *FIF*-interface with $\varphi \neq 0$. Quasiparticle Andreev interface states with the spectra of Eqs. (2), (3) are characterized by a nontrivial spin structure, which substantially depends (together with the spectra themselves) on φ, Θ and D. In general, each of the two incoming and two outgoing parts of quasiparticle trajectories, forming an Andreev interface state, has its own specific spin polarization. This should be compatible with no spin current they carry, on the whole, across the interface. Figs. 1 and 2 demonstrate the evolution of spectra and spin polarizations of four branches of Andreev interface states as functions of Θ in tunnel junctions (with transparency $D = 0.1$) and highly transparent junctions ($D = 0.95$) respectively. Two particular relative orientations of magnetization $\varphi = 0.1\pi$ (left column) and $\varphi = 2\pi/3$ (right column) are chosen. For definiteness, we consider spin polarizations of Andreev states on the incoming part of the quasiparticle trajectory in the right superconductor. The spin polarization gradually changes with the parameter Θ in all cases considered. A characteristic scale of Θ for the spin reconstruction diminishes with decreasing the misorientation angle φ. For vanishing φ the scale vanishes and there are abrupt jumps from parallel to antiparallel (or vice versa) spin orientations with respect to the magnetization, taking place at those values of Θ, where $\varepsilon_i(\Theta) = \pm\Delta$ [15].

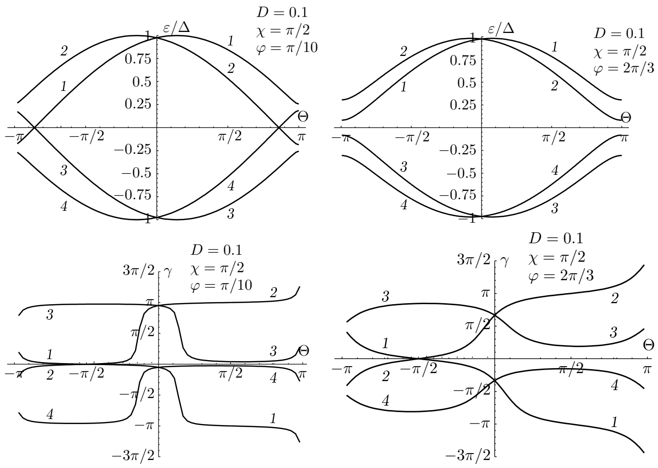

FIG. 1: Upper panel: Energies of the four branches of Andreev interface states as functions of Θ. Lower panel: Angle $\gamma(\Theta)$ of the spin of an incoming quasiparticle in the right superconductor with the magnetization of the right ferromagnetic layer, for each of the four branches of the Andreev interface states. Left column: $\varphi = 0.1\pi$. Right column: $\varphi = 2\pi/3$. Transparency and phase difference have values $D = 0.1$ and $\chi = \pi/2$, respectively.

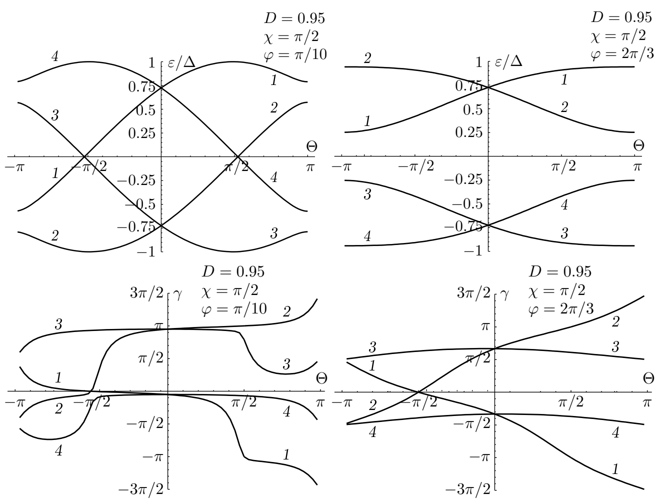

FIG. 2: The same as in Fig. 1 for highly transparent junctions with $D = 0.95$.

Only in the particular case $\varphi = 0$, when a single magnetization direction is present inside a symmetric magnetic interface, each of the Andreev interface states possesses, as a whole, a definite spin-up or spin-down polarization, identical for all incoming and outgoing quasiparticle trajectories forming the state. Then the spectra of the spin-up polarized Andreev bound states are [15]: $\varepsilon^{\uparrow}_{1,2} = |\Delta| \operatorname{sgn}\left(\sin \dfrac{\Phi_{1,2}(\chi, \Theta, \varphi = 0)}{2}\right) \cos \dfrac{\Phi_{1,2}(\chi, \Theta, \varphi = 0)}{2}$. The energies $\varepsilon^{\downarrow}_{1,2}$ for spin-down Andreev bound states are obtained from $\varepsilon^{\uparrow}_{1,2}$ by substituting $\Theta \to -\Theta$.

The spectra of Andreev states and their spin polarizations as functions of the misorientation angle φ are shown in Fig. 3. The spin polarization at $\varphi \neq 0$ makes a finite angle with both magnetization directions and differs on different incoming and outgoing trajectories related by the bound state. As already mentioned above, for antiparallel magnetizations ($\varphi = \pi$) the spectra are doubly degenerated. Spin polarizations, shown in Fig. 3 for $\varphi = \pi$, can be considered as correct eigenfunctions in zeroth order approximation in small deviations $\varphi - \pi$.

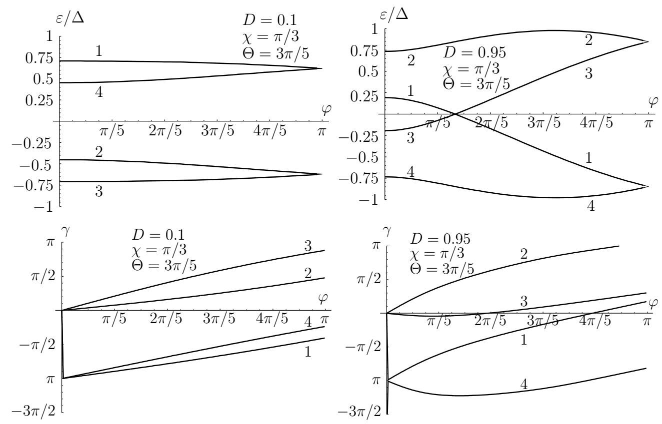

FIG. 3: Upper panel: Energies of the four branches of Andreev interface states as functions of misorientation angle φ. Lower panel: Angle $\gamma(\varphi)$ of the spin of an incoming quasiparticle in the right superconductor with the magnetization of the right ferromagnetic layer, for each of four branches of the Andreev interface states. Left (right) column: $D = 0.1$ ($D = 0.95$). The phase difference is $\chi = \pi/3$, and $\Theta = 3\pi/5$.

The spin structure of Andreev interface states at nonzero φ should be taken into account in producing nonequilibrium occupation of the states. For $\varphi = 0$ only the interlevel transitions accompanied with spin-flip processes are possible under certain conditions [15]. On account of the complicated spin structure of the Andreev states at nonzero φ, there are actually no strict restrictions to a change of quasiparticle spin in the transition.

The Josephson current is carried by the bound states (2), analogously to the situation in nonmagnetic symmetric junctions [23, 24, 25, 26]. Hence, in a quantum point contact with a *FIF* constriction the total Josephson current carried by four Andreev states (2) can be found as $J(\chi, T) = 2e \sum\limits_{m} \dfrac{d\varepsilon_m}{d\chi} n(\varepsilon_m) = -2e \sum\limits_{\varepsilon_m > 0} \dfrac{d\varepsilon_m}{d\chi} \tanh \dfrac{\varepsilon_m}{2T}$. It is not difficult to calculate the current in this scheme numerically. The Josephson critical current as a function of the misorientation angle φ, normalized to its value at $\varphi = 0$, is shown in Fig. 4 for various Θ and for two values of the transparency $D = 0.01,\ 0.8$ (the upper and the lower panels respectively) and the temperature $T = 0.1T_c,\ 0.8T_c$ (the right and the left columns).

We define the critical current as a positive quantity, as it is usually determined experimentally. There are

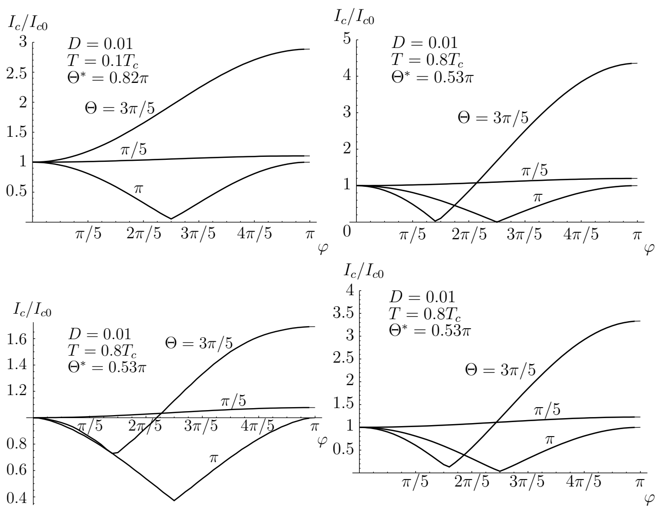

FIG. 4: Critical current as a function of the misorientation angle φ, normalized to its value at $\varphi = 0$. In the particular case $\varphi = 0$ the 0-π transition takes place for $\Theta > \Theta^*(T, D)$.

two qualitatively different regimes for the behavior of the Josephson critical current as a function of φ in all particular cases displayed in Fig. 4. The two regimes are separated by a characteristic value $\Theta^*(T, D)$, which depends on the temperature and the transparency. For $\Theta < \Theta^*$ the current is a monotonous function of the misorientation angle, reaching the maximum for the antiparallel orientation of the magnetizations. For $\Theta > \Theta^*$ the current manifests, however, a nonmonotonic dependence on the misorientation angle with well pronounced minimum at some intermediate value of φ and the maximum at $\varphi = \pi$. In the case $\Theta = \pi$ the currents at $\varphi = 0$ and $\varphi = \pi$ are equal to each other. The parameter Θ^* admits a simple physical interpretation, associated with the junction at $\varphi = 0$. At zero misorientation angle the junction acquires a uniformly oriented ferromagnetic interface. Then the Josephson current is equivalent to that studied in [8, 12, 13, 15]. It can be shown, that for $\varphi = 0$ and $\Theta = \Theta^*(T, D)$ the $0 - \pi$ transition takes place in the junction just at the given temperature T. Hence, for $\Theta > \Theta^*(T, D)$ the equilibrium state of the junction with $\varphi = 0$ is the π-state, while for $\Theta < \Theta^*(T, D)$ it is the 0-state. We omit an analytical analysis of the total Josephson current in the case $\varphi = 0$, since the results exactly coincide with those obtained in Refs. 13, 15.

Furthermore, there is no $0-\pi$ transition in the junction with antiparallel magnetization, $\varphi = \pi$, in the three-layer interface. Indeed, it is straightforward to get from Eq. (2) the Josephson current in the particular case $\varphi = \pi$:

$$J(\chi, T) = \frac{eD|\Delta| \sin\chi}{\sqrt{D\cos^2\frac{\chi}{2} + R\cos^2\frac{\Theta}{2}}} \times$$

$$\times \tanh \frac{|\Delta|\sqrt{D\cos^2\frac{\chi}{2} + R\cos^2\frac{\Theta}{2}}}{2T} \,. \qquad (5)$$

In contrast to the case $\varphi = 0$, the current (5) does not change its sign at any temperature. The same assertion is valid also for junctions with dirty superconductors, where Andreev states are fully destroyed [10, 16]. We conclude, that the nonmonotonic dependence of the Josephson current on φ arises due to the $0 - \pi$ transition taking place with varying the misorientation angle at an intermediate value of φ. This always occurs under the condition that there is a π-junction at $\varphi = 0$. If one defined the critical current in the π-junction as the negative quantity, then the nonmonotonic behavior would transform into the monotonic one, accompanied with a change of sign and discontinuity whenever $\min |J_c| \neq 0$.

The dependence of the Josephson current on the misorientation angle φ becomes especially simple and clear in the tunneling limit. In tunnel quantum point contacts the Josephson current takes the form $J(T, \varphi, \chi) = J(T, \varphi)\sin\chi$, where

$$J(T, \varphi) = J^{(p)}(T)\cos^2\frac{\varphi}{2} + J^{(a)}(T)\sin^2\frac{\varphi}{2} \,, \qquad (6)$$

$$J^{(p)}(T) = eD|\Delta| \left[\cos\frac{\Theta}{2}\tanh\left(\frac{|\Delta|\cos\frac{\Theta}{2}}{2T}\right) - \right.$$
$$\left. - \frac{|\Delta|}{2T}\frac{\sin^2\frac{\Theta}{2}}{\cosh^2\left(\frac{|\Delta|\cos\frac{\Theta}{2}}{2T}\right)}\right], \qquad (7)$$

$$J^{(a)}(T) = \frac{eD|\Delta|}{\cos\frac{\Theta}{2}}\tanh\left(\frac{|\Delta|\cos\frac{\Theta}{2}}{2T}\right) \,. \qquad (8)$$

The quantities $J^{(p)}(T)$, $J^{(a)}(T)$ are defined as $J^{(p)}(T) \equiv J(T, \varphi = 0)$, $J^{(a)}(T) \equiv J(T, \varphi = \pi)$, so that $|J^{(p)}(T)|$, $|J^{(a)}(T)|$ are critical currents in tunnel junctions with parallel and antiparallel orientations of the exchange fields in the three-layer interface. The dependence (6) on the misorientation angle has been derived in the tunneling limit earlier in Ref. 11, disregarding the contribution from Andreev states and, hence, the $0 - \pi$ transition. As one can conclude from (6), the $0-\pi$ transition can take place with varying φ, if $J_c^{(p)}(T)$ and $J_c^{(a)}(T)$ have opposite signs. This is exactly the reason for a nonmonotonic dependence of the critical current on φ to show up. Eq. (6) is quite general within the tunneling limit and not applicable to highly transparent junctions. Spin polarizations of the eigenstates on any side of the impenetrable interface are aligned parallel or antiparallel to the respective magnetization direction. Making the projections of the spin polarized states from one side on

the eigenstates on another side (with the spin polarization rotated by the angle φ with respect to the initial one), one confirms in the tunneling limit that the current is of the form (6).

In conclusion, we have investigated theoretically spectra and spin structures of interface Andreev states in *S-FIF-S* junctions. Both finite transparency and the misorientation angle between in-plane magnetizations of ferromagnetic layers were taken into account. We demonstrated that the Josephson critical current as a function of the misorientation angle always manifests a nonmonotonic behavior, if at $\varphi = 0$ the equilibrium state of the quantum point contact is the π-state.

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